MATERIAL CHARACTERIZATION OF POLYCRYSTALS THROUGH HYPERSPACE

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Summary The Voronoi tessellation technique in hyperspace is applied to the material characterization of polycrystals. Once Voronoi polytopes in four dimensions are projected to three-dimensional space, the volume and morphology reveal much variation. The inhomogeneity forces are evaluated both in cell level and in interfacial level without any periodicity. Particularly the effect of small cells on the surrounding is evaluated, through which the randomness in polycrystalline aggregate is discussed.

INTRODUCTION

Polycrystalline materials are composed of great amount of crystals whose shape and dimension are almost random. Such randomness has a dominant influence on the material inhomogeneity, which is a cause of damage and failure in polycrystalline aggregate. In order to characterize the material behaviour from the computational mechanics viewpoint, we have to take account of the randomness in shape and dimension. However, the conventional technique by the Voronoi tessellation, which may be the most promising method to generate complex polyhedrons, provides insufficient morphology in terms of volume distribution.

A rational extension is made on the modelling of polycrystalline material. The Voronoi tessellation is carried out in hyperspace of four dimensions, and the resulting polychorons, i.e. 4-D polytopes, are projected into three-dimensional space. This makes the polyhedrons maintain strictly convex and the volume distribution vary in the 3-D domain. Applying this procedure to the finite element method, we evaluate the material inhomogeneity. We discuss the development of inhomogeneity force with particular interest in the damage evolution around material surface.

POLYCRYSTALLINE MATERIAL MODEL

Polycrystalline materials involve crystals, hereafter simply called “cells”, with a variety of shape and dimension. In order to generate an aggregate of such cells within the framework of computational geometry, we employ an algorithm called “Voronoi tessellation” technique. This technique proceeds to find the closest mid-planes relative to grids, which are randomly distributed in a proper space [1], and the polytopes through this procedure are strictly convex. From physical point of view, the 3-D Voronoi tessellation can be referred to the growth of cells at constant growth rate. However, it is well known that, when setting grids at random in three-dimensional space, the volumes of the polytope have poor variation. In order to overcome this problem, we extend the procedure to the hyperspace of four dimensions. This states that the growth of cells is also govern by an additional degree of freedom. This degree could be referred to anything else, e.g. time.

Let $[x_i, y_i, z_i, w_i]$ be components of an i-th grid and then $[x_i, y_i, z_i, -w_i]$ be its mirror on w-axis. Apparently the “mid-plane” is chosen as w=0 (if it is the closest), and this “plane” actually constitutes a 3-D polytope. Here we can control the variation of volume by setting the value of w_i, which is also advantageous in other applications. Since the polytope is strictly convex in 4-D, it also holds true in 3-D. This convexity property takes numerous advantages in coding the algorithm for finite element mesh division. Figure 1 demonstrates an example of polycrystalline aggregate through this procedure, in which cells are separated in display for convenience. It is found that some cells inside the domain are small and others are large. Such a variety cannot be achieved by the conventional 3-D Voronoi tessellation. This technique can be used even for generating inclusions and precipitates in polycrystalline aggregates.

In order to examine the variety of volume in individual cells, the distribution of cell volumes is plotted in Figure 2 where the distribution by the conventional 3-D technique is also shown for comparison. 100 cells are generated in a unit cube of 1mm^3, although it is essentially dimensionless. And cells inside the domain, i.e. excluding the ones facing external surfaces, are picked up and examined for eight types of different cell patterns. The average of volumes is then mostly 0.01mm^3. We have totally 196 cells in the 3-D patterns and 206 cells in the 4-D patterns. As is mentioned above, the distribution by the 3-D technique reveals a clear peak around the volume average. In contrast the volume distribution is flat by the 4-D technique. This means that a variety of cells in volume exist in the representative cube. It follows that we can generate more realistic polycrystalline aggregate model. The cells are sub-divided into 10-node tetrahedral elements and the model is applied to the finite element analysis.

INHOMOGENEITIES IN MODEL MATERIAL

An anisotropic constitutive model is adopted in the simulation, where random orientations are given in each cell. Figure 3 demonstrates an example of stress distribution of sample cube. Stresses and strains vary within the local portions, even when a simple tension is loaded. Particularly remarkable stress concentrations can be observed around (a) triple point of cells and (b) particular interfaces. In order to evaluate this non-uniformity, we examine the inhomogeneity concept [2,3]. The inhomogeneity force $\boldsymbol{f}^{\mathrm{inh}}$ is given by

$$\int \boldsymbol{f}^{\text{inh}} dV = \int \boldsymbol{b}^{\mathrm{T}} \boldsymbol{N}\, dS\,, \tag{1}$$

where $\boldsymbol{b}$ is called Eshelby stress defined as $\boldsymbol{b}=W\boldsymbol{1}-\boldsymbol{TF}$. W stands for the energy density, $\boldsymbol{T}$ is the first Piola-Kirchhoff stress, and $\boldsymbol{F}$ means the deformation gradient. Figure 4 shows the relationship between the norm of inhomogeneity force and the misfit of two neighbouring cells. The inhomogeneity force develops according to the deformation. A slight tendency is obtained between the misfit and the inhomogeneity force and larger forces are generated around the surface. We point out that further large values appear around small size cells irrelevant to the misfit.

CONCLUSIONS

In order to idealize the polycrystalline aggregate, we propose a methodology to generate convex cells with various volumes by use of the Voronoi tessellation technique in hyperspace. This method is quite simple but robust because of the cell convexity. Applying this to the finite element schemes, we examine the material inhomogeneity of the model material. It is shown that the randomness in crystal morphology gives a predominant influence on the non-uniformity of deformation in microscopic level.

References

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[2] Maugin G.A.: Material Inhomogeneities in Elasticity. Chapman & Hall, London 1993.
[3] Kienzler R., Hermann G.: Mechanics in Material Space, Springer, Berlin, 2000.

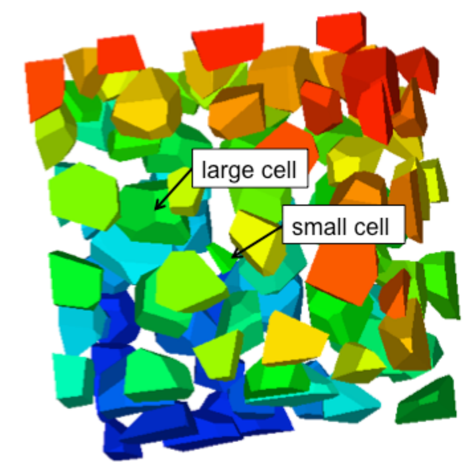

Figure 1. Cell distribution by 4-D Voronoi tessellation.

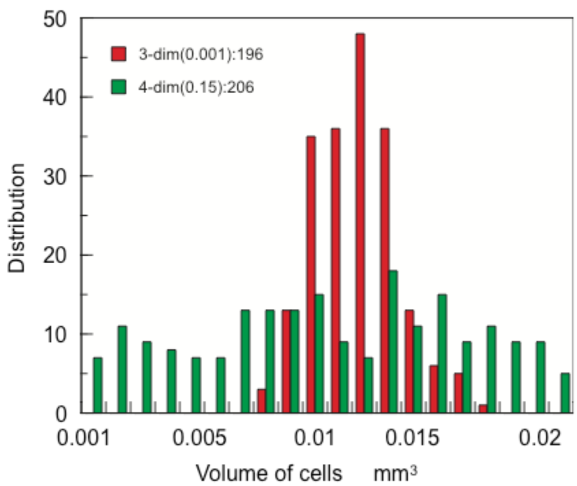

Figure 2. Comparison of volume distribution of cells.

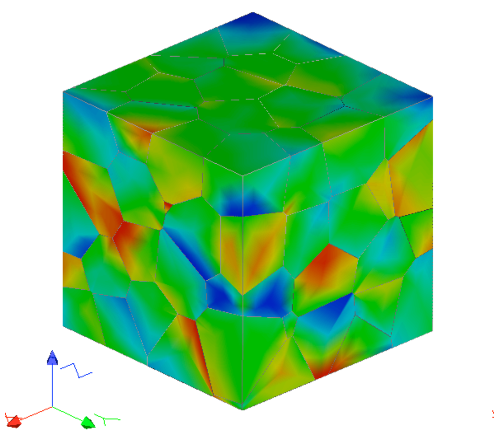

Figure 3. Example of stress distribution.

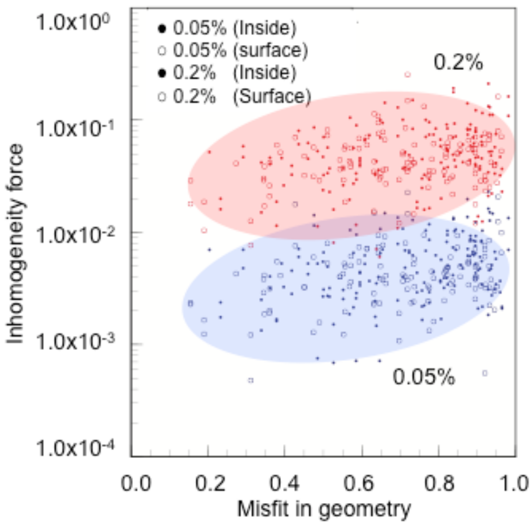

Figure 4. Correlation between inhomogeneity force and misfit.